Fig. 1

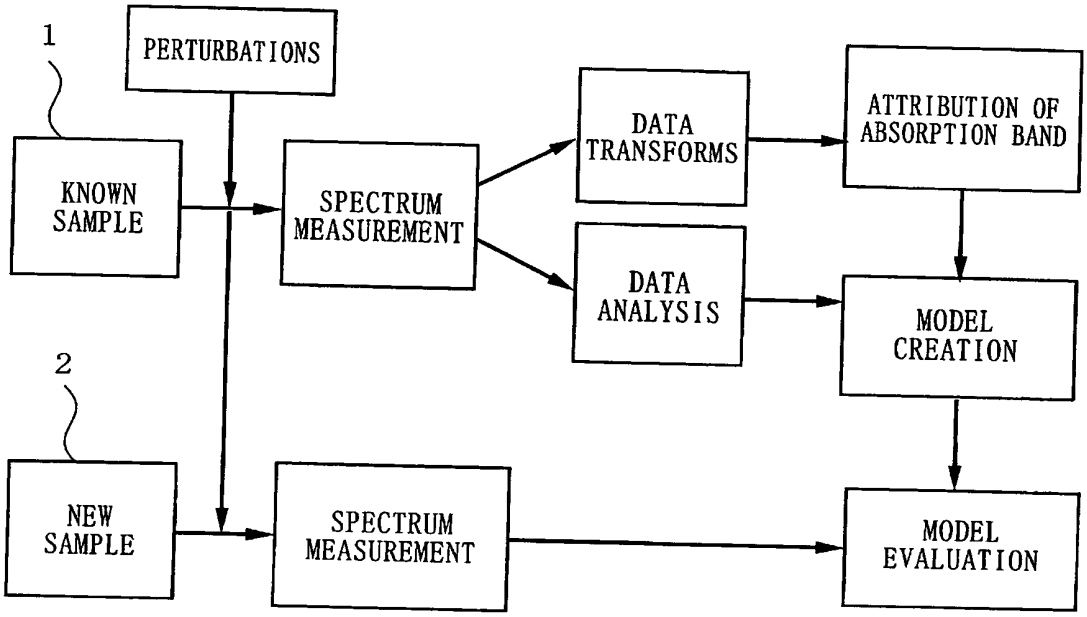

1
PERTURBATIONS
KNOWN SAMPLE
SPECTRUM MEASUREMENT
DATA TRANSFORMS
ATTRIBUTION OF ABSORPTION BAND
DATA ANALYSIS
MODEL CREATION
2
NEW SAMPLE
SPECTRUM MEASUREMENT
MODEL EVALUATION

Fig. 2

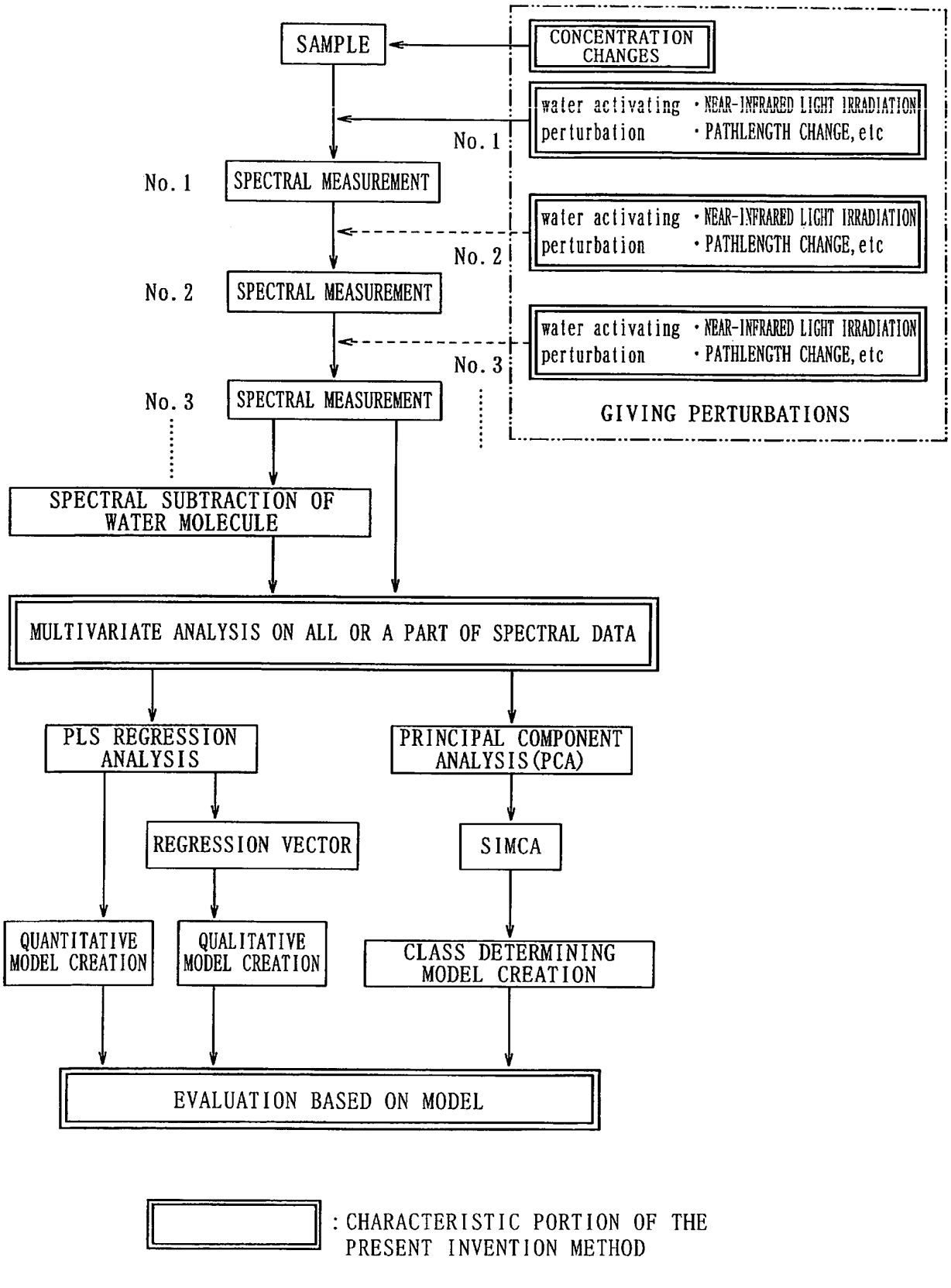

SAMPLE
CONCENTRATION CHANGES
water activating perturbation
・NEAR-INFRARED LIGHT IRRADIATION
・PATHLENGTH CHANGE, etc
No. 1
No. 1
SPECTRAL MEASUREMENT
water activating perturbation
・NEAR-INFRARED LIGHT IRRADIATION
・PATHLENGTH CHANGE, etc
No. 2
No. 2
SPECTRAL MEASUREMENT
water activating perturbation
・NEAR-INFRARED LIGHT IRRADIATION
・PATHLENGTH CHANGE, etc
No. 3
No. 3
SPECTRAL MEASUREMENT
GIVING PERTURBATIONS
SPECTRAL SUBTRACTION OF WATER MOLECULE
MULTIVARIATE ANALYSIS ON ALL OR A PART OF SPECTRAL DATA
PLS REGRESSION ANALYSIS
PRINCIPAL COMPONENT ANALYSIS (PCA)
REGRESSION VECTOR
SIMCA
QUANTITATIVE MODEL CREATION
QUALITATIVE MODEL CREATION
CLASS DETERMINING MODEL CREATION
EVALUATION BASED ON MODEL
: CHARACTERISTIC PORTION OF THE PRESENT INVENTION METHOD

Fig. 3

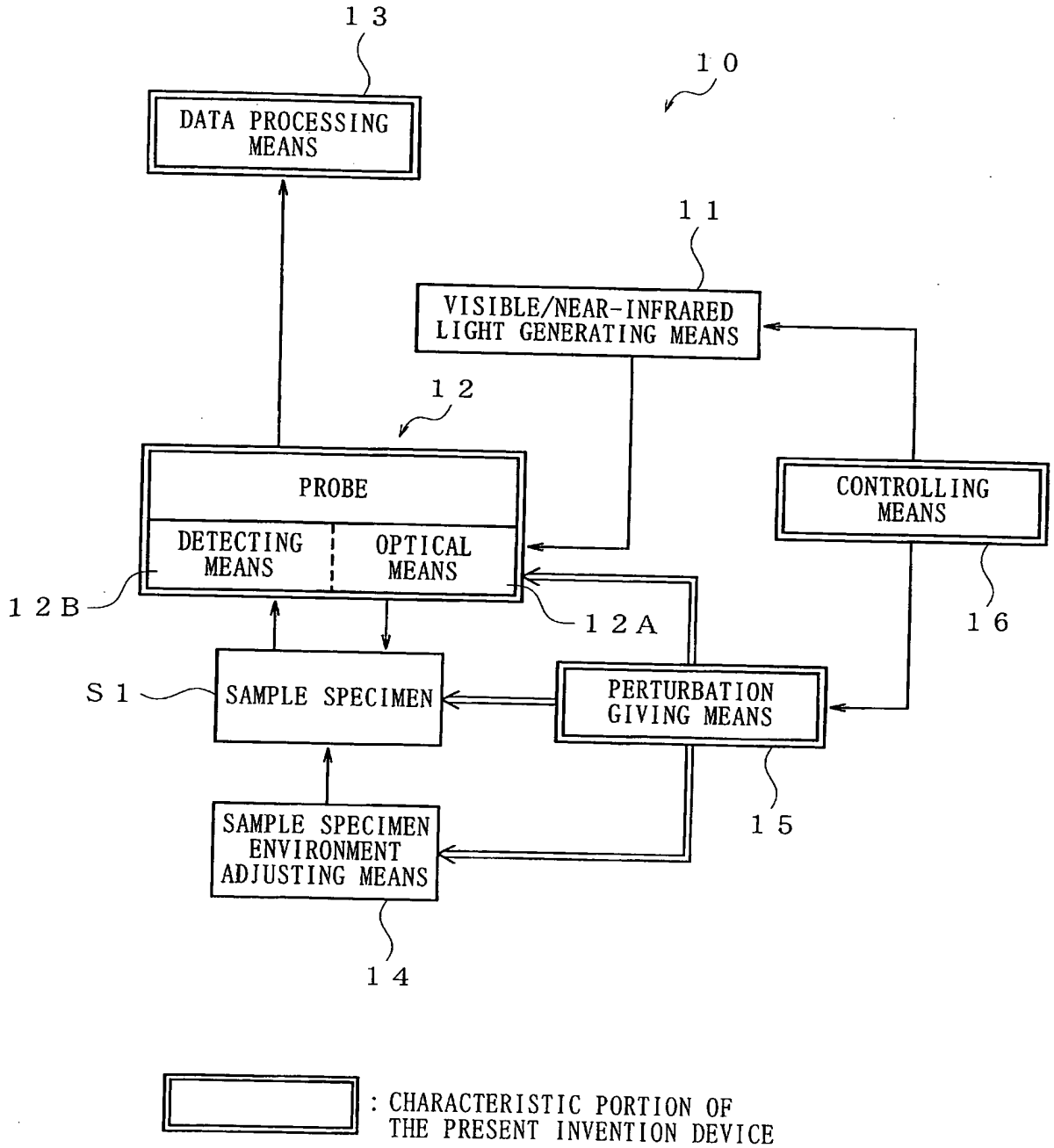

13
10
DATA PROCESSING MEANS
11
VISIBLE/NEAR-INFRARED LIGHT GENERATING MEANS
12
PROBE
DETECTING MEANS
OPTICAL MEANS
CONTROLLING MEANS
12B
12A
16
S1
SAMPLE SPECIMEN
PERTURBATION GIVING MEANS
15
SAMPLE SPECIMEN ENVIRONMENT ADJUSTING MEANS
14
: CHARACTERISTIC PORTION OF THE PRESENT INVENTION DEVICE

Fig. 4

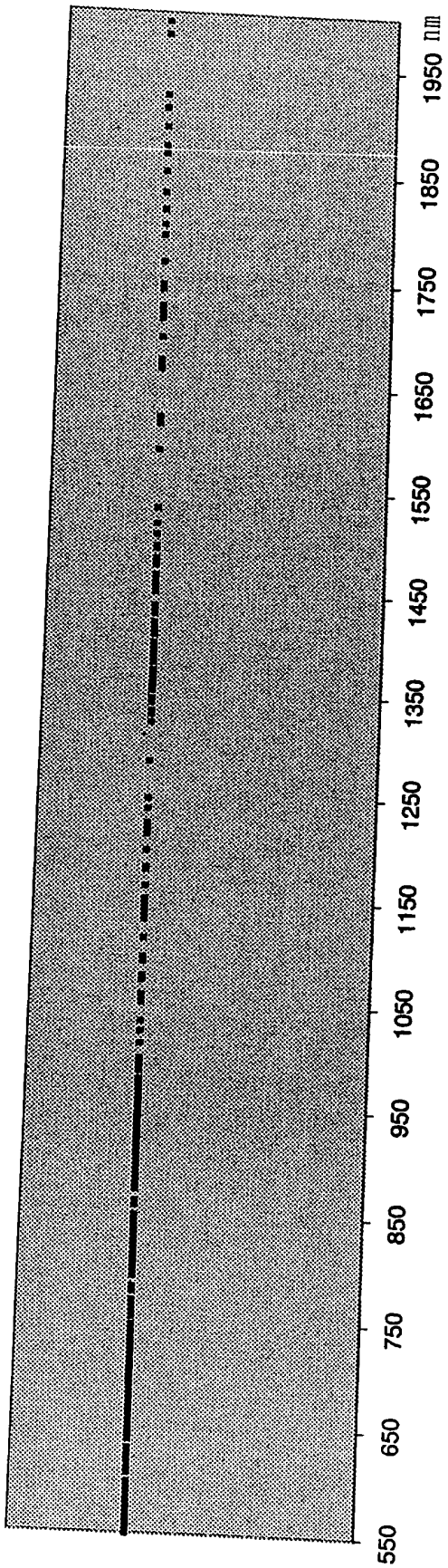
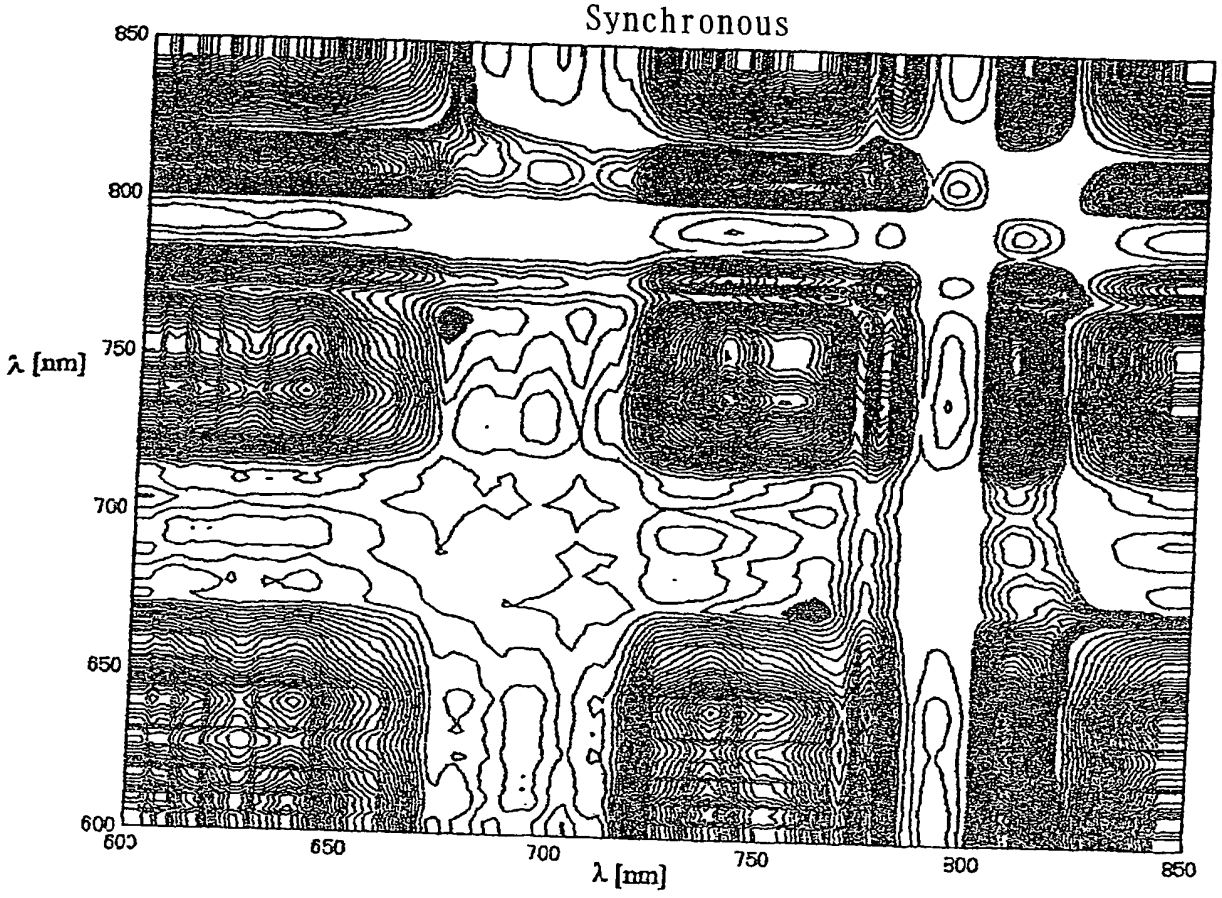

550
650
750
850
950
1050
1150
1250
1350
1450
1550
1650
1750
1850
1950 nm

Fig. 5

Autopeaks: 606 nm, 628 nm, 640 nm, 678 nm, 738 nm, 750 nm, and 776 nm



2D-COS synchronous map, crosspeaks

Fig. 6

Autopeaks: 606 nm, 628 nm, 640 nm, 678 nm, 738 nm, 750 nm, and 776 nm

Synchronous

λ [nm] x axis	λ [nm] y axis						
606	640	738	808				
610	738						
618	694						
628	770						
640	606	678	738	752	776	792	808
678	624	632	638-644				
688	672						
694	614	618	730	810			
696	730	810					
704	764						
710	624	632	642	808			
738	606	610	640	752	776	792	808
752	640	738					
770	628						
772	764						
776	610	640	738	792	810		
792	606	610	640	738	776	808	
808	606	640	694	738	776	792	
810	640	678	680	682	694	738	776

2D-COS synchronous map, crosspeaks

Fig. 7

RESULT OF MEASUREMENT

RAW SPECTRA AND NOISE RANGE

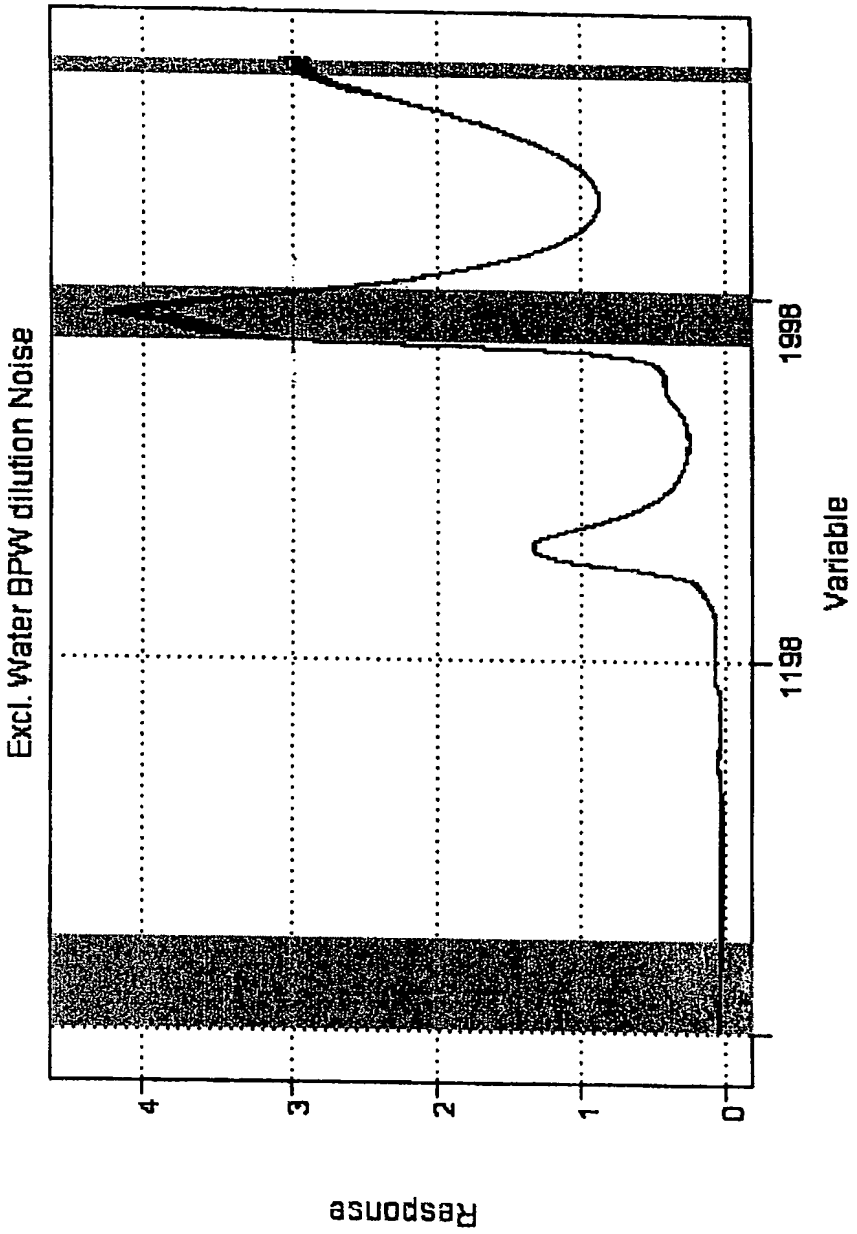
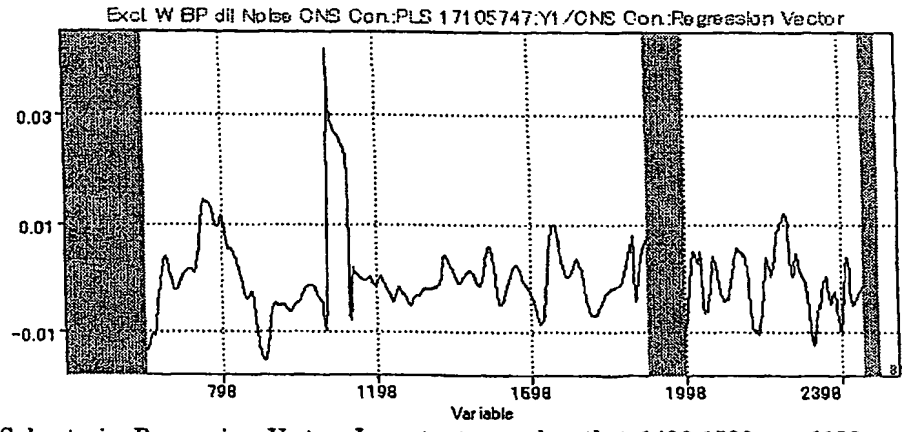
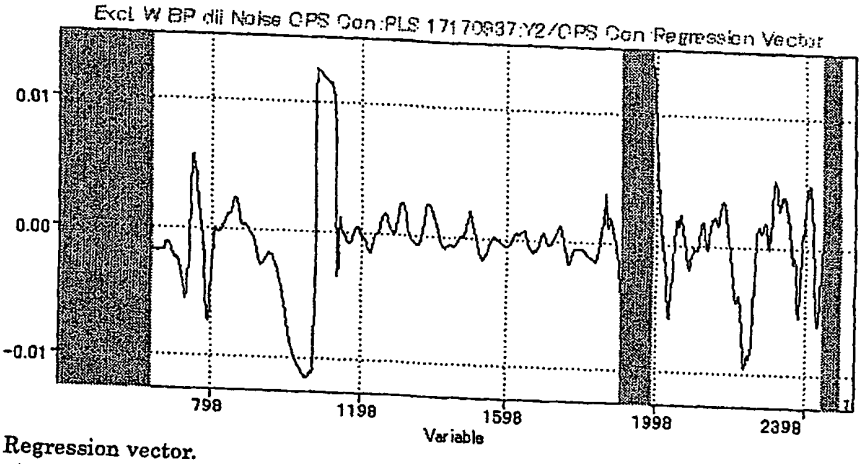


Fig. 8



CNS bacteria Regression Vector. Important wavelengths: 1406-1500nm, 1180nm-1306nm

Fig. 9



CPS Regression vector.
Important wavelengths: 740nm, 770nm, 808nm, 1156-1198nm, 1466nm, 1476nm, 1650nm, 1686nm, 1704nm, 1720nm, 1750nm, 1846nm, 1890nm

Fig. 10

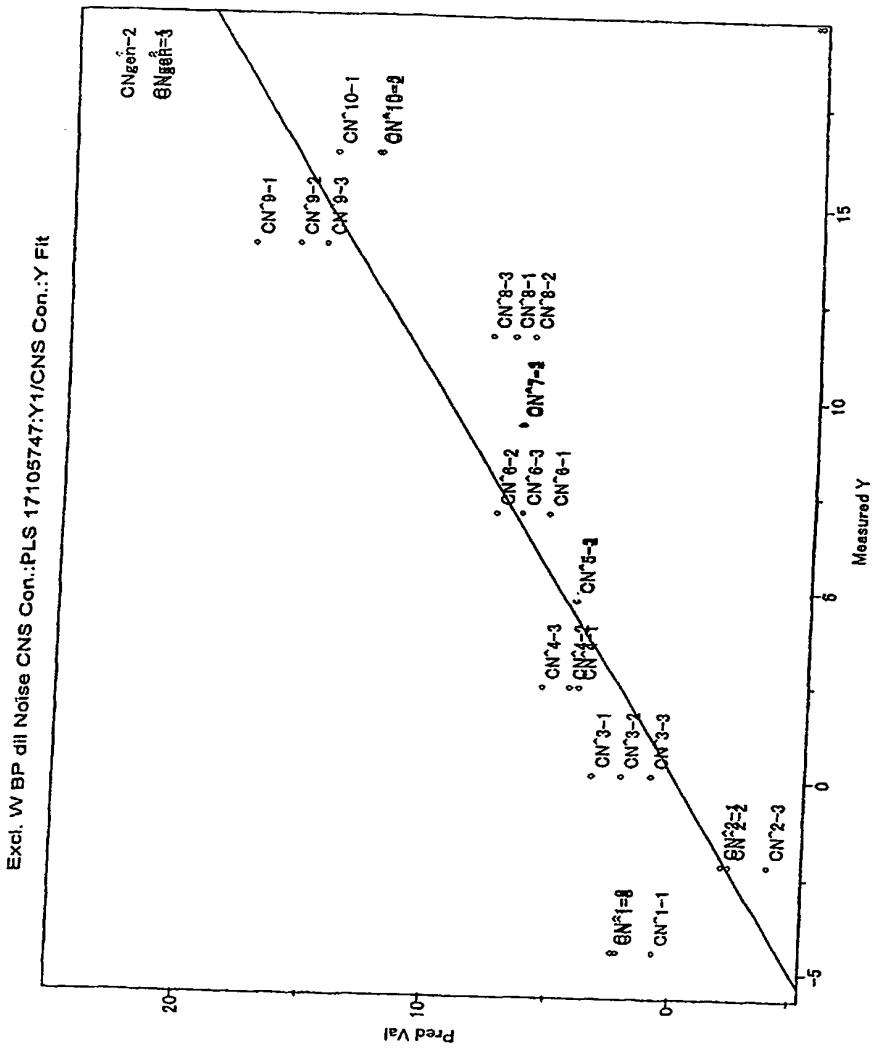

Excl. W BP dil Noise CNS Con.:PLS 17105747:Y1/CNS Con.:Y Fit
Pred Val
Measured Y
20
10
0
-5
0
5
10
15
CN^9-1
CN^9-2
CN^9-3
CN^10-1
CN^8-3
CN^8-1
CN^8-2
CN^6-2
CN^6-3
CN^6-1
CN^4-3
CN^3-1
CN^3-3
CN^1-1
CN^2-3

Fig. 11

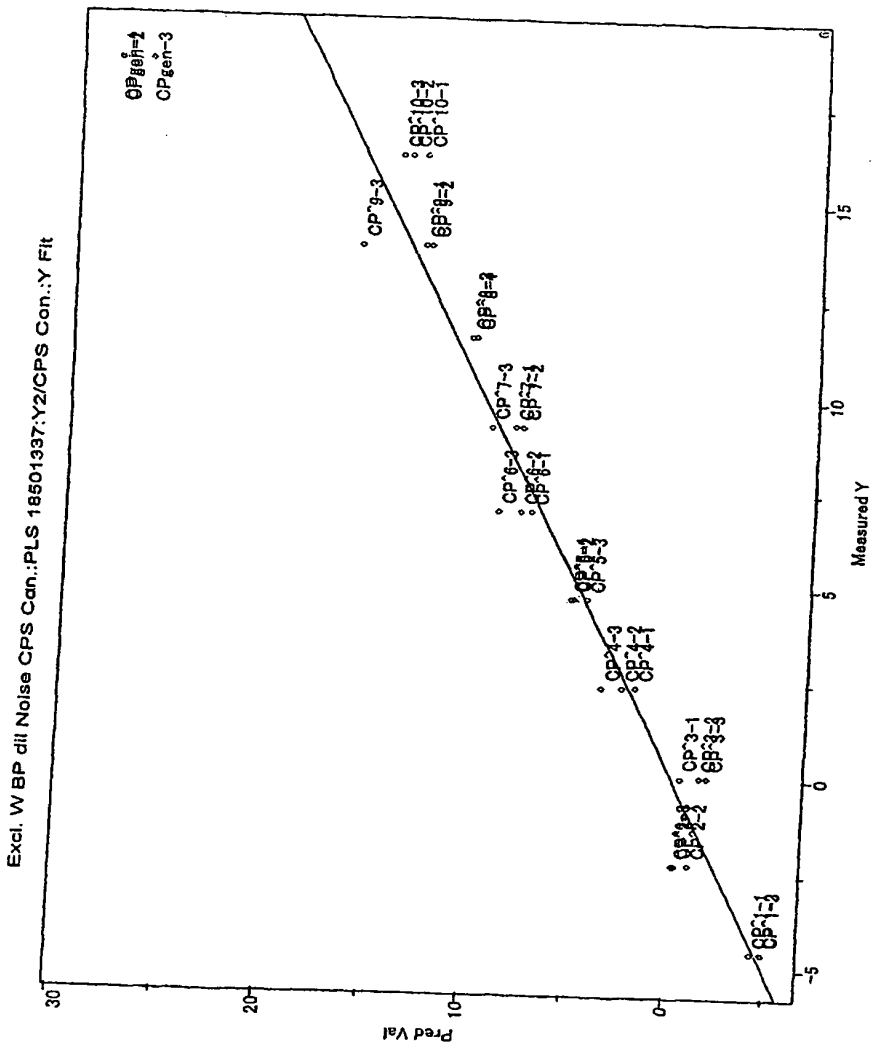
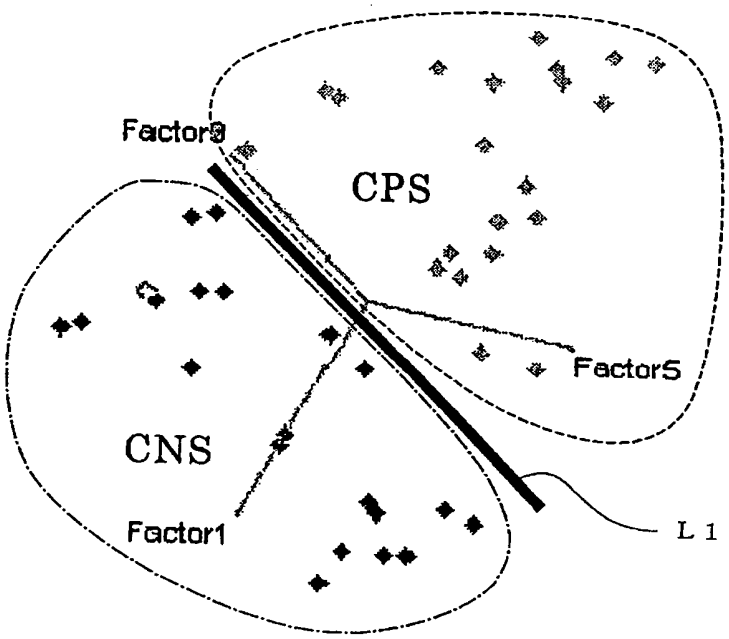

Excl. W BP dil Noise CPS Can.:PLS 18501337:Y2/CPS Con.:Y Fit
Pred Val
Measured Y
30
20
10
0
-5
0
5
10
15

Fig. 12

CPS								
	Percent	cumulative	SEV	Press Val	r Val	SEC	Press Cal	r Cal
Factor6	0.952331	97.56091	3.096218	316.3566	0.944926	0.674208	11.81845	0.996617
CNS								
	Percent	cumulative	SEV	Press Val	r Val	SEC	Press Cal	r Cal
Factor 9	0.000002	99.99999	3.04932	306.8456	0.909211	0.638169	9.774219	0.997202

Fig. 13



THREE-DIMENSION SCORE PLOT
PCA PRINCIPAL COMPONENT

Fig. 14

(a)

RESULT OF SIMCA ANALYSIS

INTERCLASS DISTANCE BETWEEN CNS AND CPS

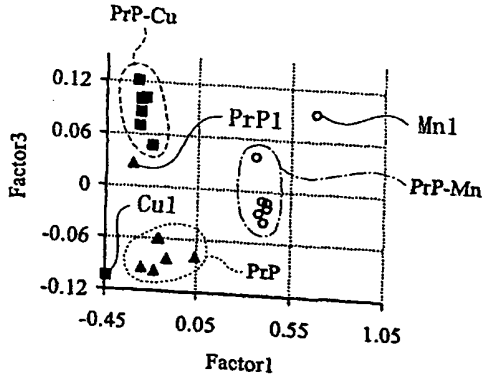
	SAMPLE • WAVELENGTH SELECTION	DISTANCE
A1	WATER EXCLUDE (Autoscale,Smooth(15),2nd Derivative(25))	0.836
A2	WATER, NOISE EXCLUDE (Autoscale,Smooth(15),1st Derivative(25))	0.823
A3	WATER, NOISE EXCLUDE (Autoscale,Smooth(15),2nd Derivative(25))	0.984
A4	WATER, BPW, NOISE EXCLUDE (Autoscale,Smooth(15),1nd Derivative(25))	1.156
A5	WATER, BPW, NOISE EXCLUDE (Autoscale,Smooth(15),2st Derivative(25))	1.826
A6	WATER, BPW, DILUTED SAMPLE, NOISE EXCLUDE, 3TIMES (Autoscale,Smooth(15),1st Derivative(25))	4.254
A7	WATER, BPW, DILUTED SAMPLE, NOISE EXCLUDE (Autoscale,Smooth(15),2nd Derivative(25))	2.103
A8	WATER, BPW, DILUTED SAMPLE, NOISE EXCLUDE, 1TIME (Autoscale,Smooth(15),1st Derivative(25))	4.132

(b)

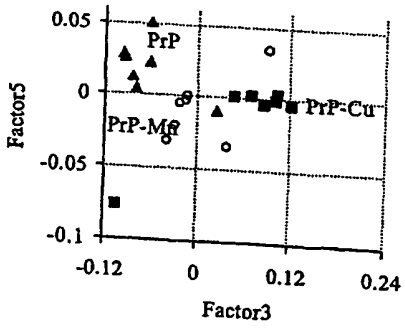
	Pred. CNS	Pred.CPS	No match
CNS	34.0000	0.0000	0.0000
CPS	0.0000	36.0000	0.0000

Fig. 15

(a)



(b)



(c)

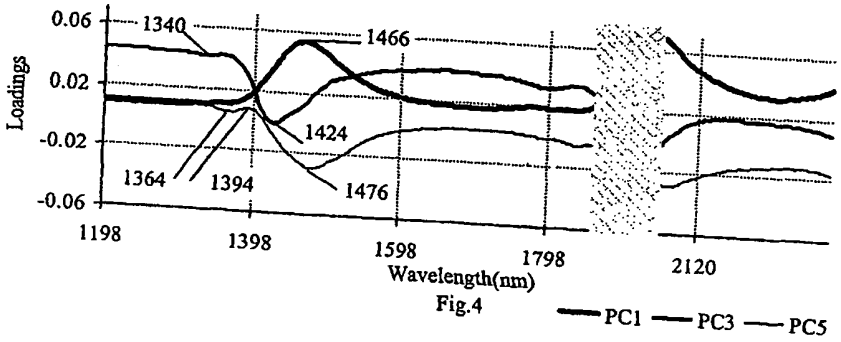


Fig.4

Fig. 16

Table 2 SIMCA Interclass Distance

	PrP-Cu	PrP-Mn	PrP
PrP-Cu	0.00	28.81	4.15
PrP-Mn	28.81	0.00	11.44
PrP	4.16	11.44	0.00

Fig. 17

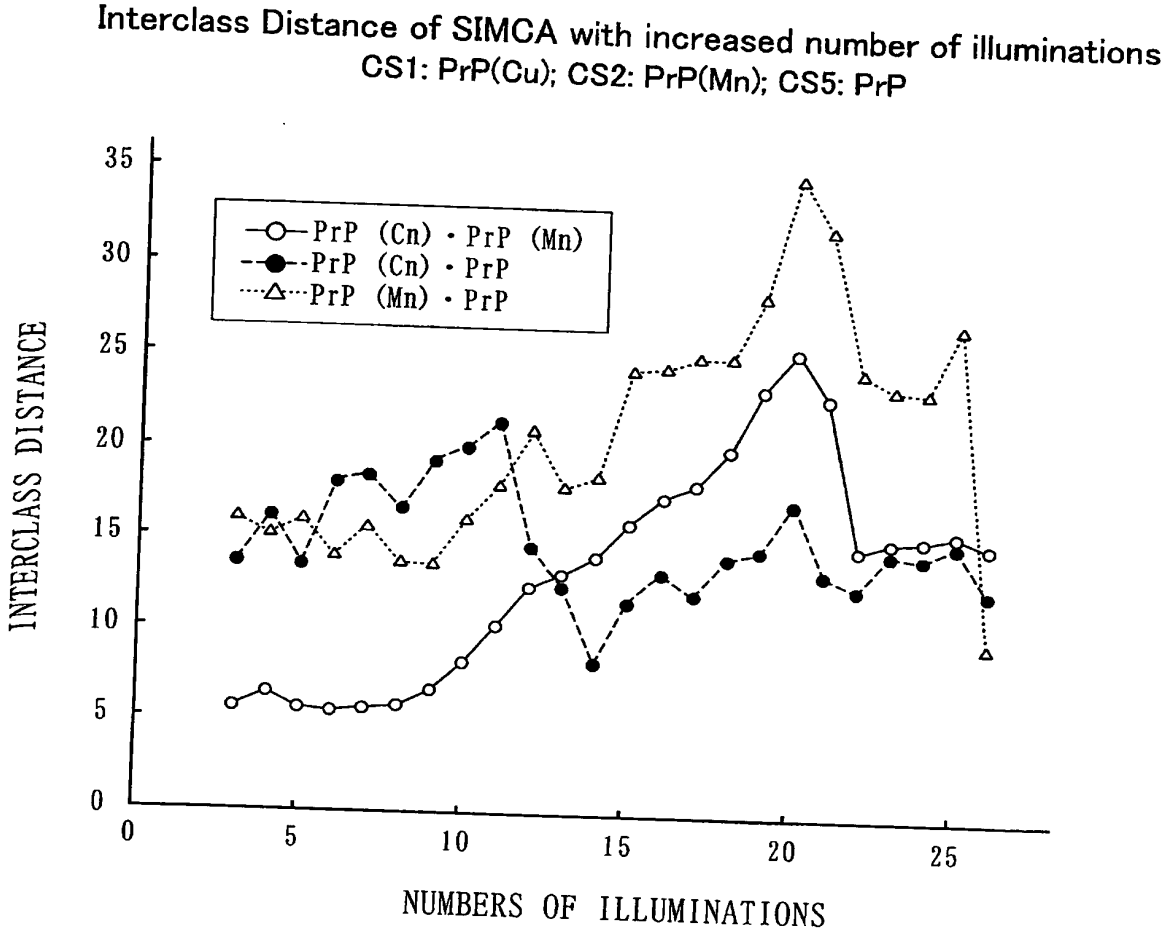

Interclass Distance of SIMCA with increased number of illuminations
CS1: PrP(Cu); CS2: PrP(Mn); CS5: PrP
PrP (Cn) · PrP (Mn)
PrP (Cn) · PrP
PrP (Mn) · PrP
INTERCLASS DISTANCE
NUMBERS OF ILLUMINATIONS
0
5
10
15
20
25
30
35

Fig. 18

SIMCA distances between PrP isomers increases when dissolved in water

	1.0 mg/ml concentrartion		
	CS2@2	CS3@1	CS4@2
CS2	0.000000	0.861595	0.652900
CS3	0.861595	0.000000	1.781953
CS4	0.652900	1.781953	0.000000

	0.5 mg/ml concentrartion		
	CS2@1	CS3@1	CS4@1
CS2	0.000000	2.434433	0.543989
CS3	2.434433	0.000000	2.806436
CS4	0.543989	2.806436	0.000000

	0.1 mg/ml concentrartion		
	CS2@2	CS3@2	CS4@1
CS2	0.000000	2.674993	1.163065
CS3	2.674994	0.000000	1.788170
CS4	1.163065	1.788170	0.000000

	0.05 mg/ml concentrartion		
	CS2@1	CS3@1	CS4@1
CS2	0.000000	7.862999	8.612659
CS3	7.862999	0.000000	5.843394
CS4	8.612659	5.843394	0.000000

CS2: PrP(Cu) in Water

CS3: PrP in Water

CS4: PrP in W(Cu) (water with cupper)

Fig. 19

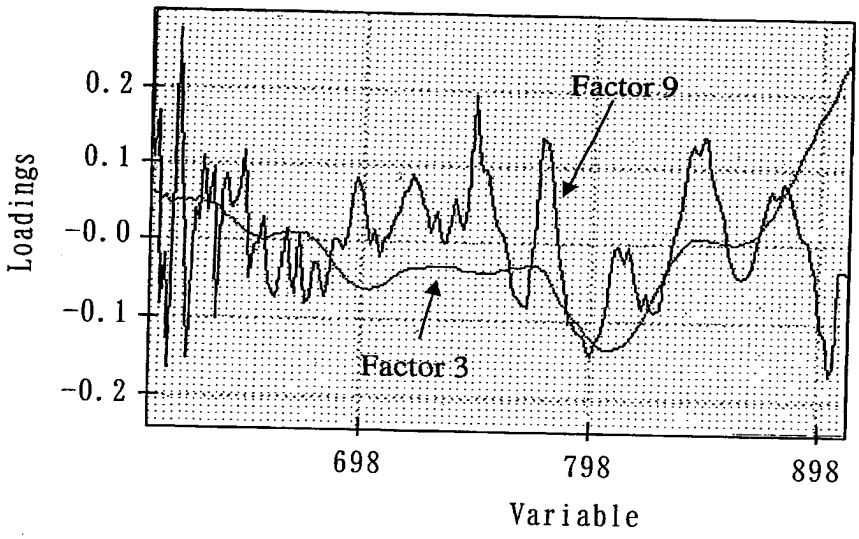
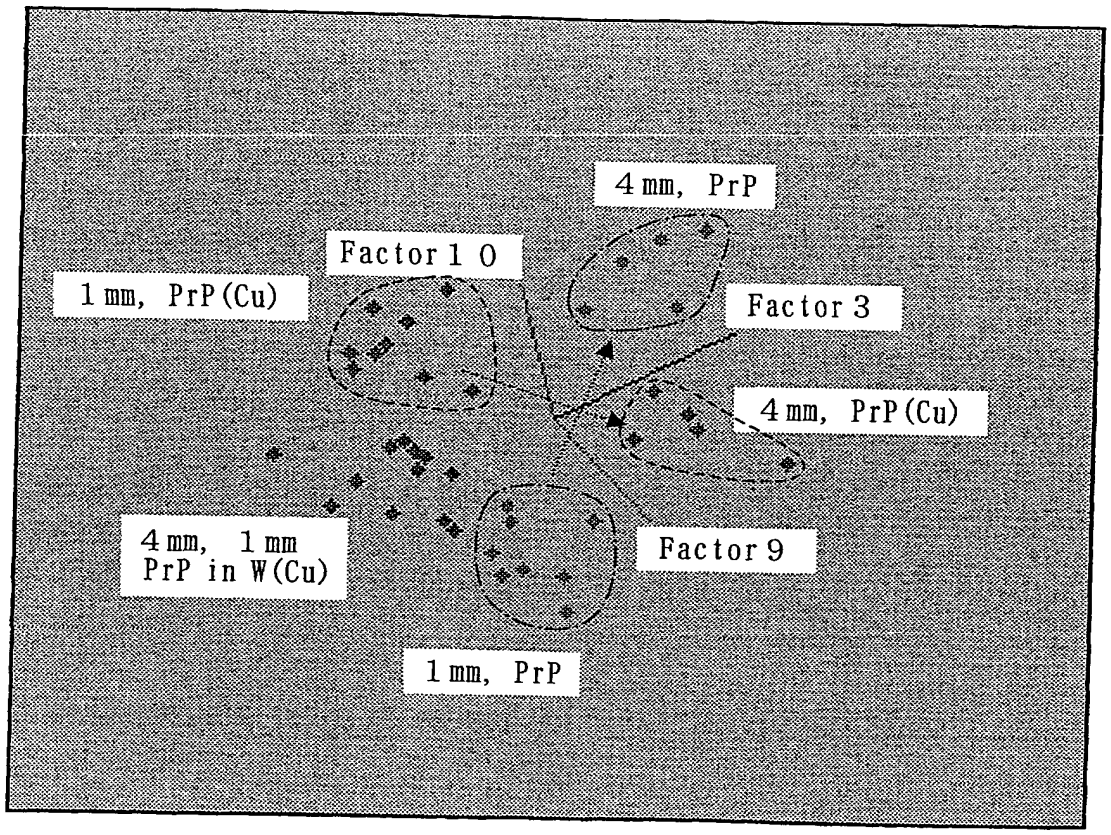


Fig. 20

(a)



(b)

Interclass Distance: SIMCA

	Class1	Class2	Class3
Class PrP(Cu) Class:1	0.0	1.19	24.84
Class PrP Class:2	1.19	0.0	26.43
Class PrP in W(Cu) Class:3	24.84	26.43	0.0

(c)

Misclassification SIMCA

	Pred1	Pred2	Pred3	No match
Actual Class 1	13.00	0.00	0.00	0.00
Actual Class 2	0.00	13.00	0.00	0.00
Actual Class 3	0.00	0.00	13.00	0.00

Fig. 21

SIMCA distances between PrP isomers increases when dissolved in water

Each PrP sample is analysed at
4 different temperatures:21℃, 30℃, 35℃, 37℃

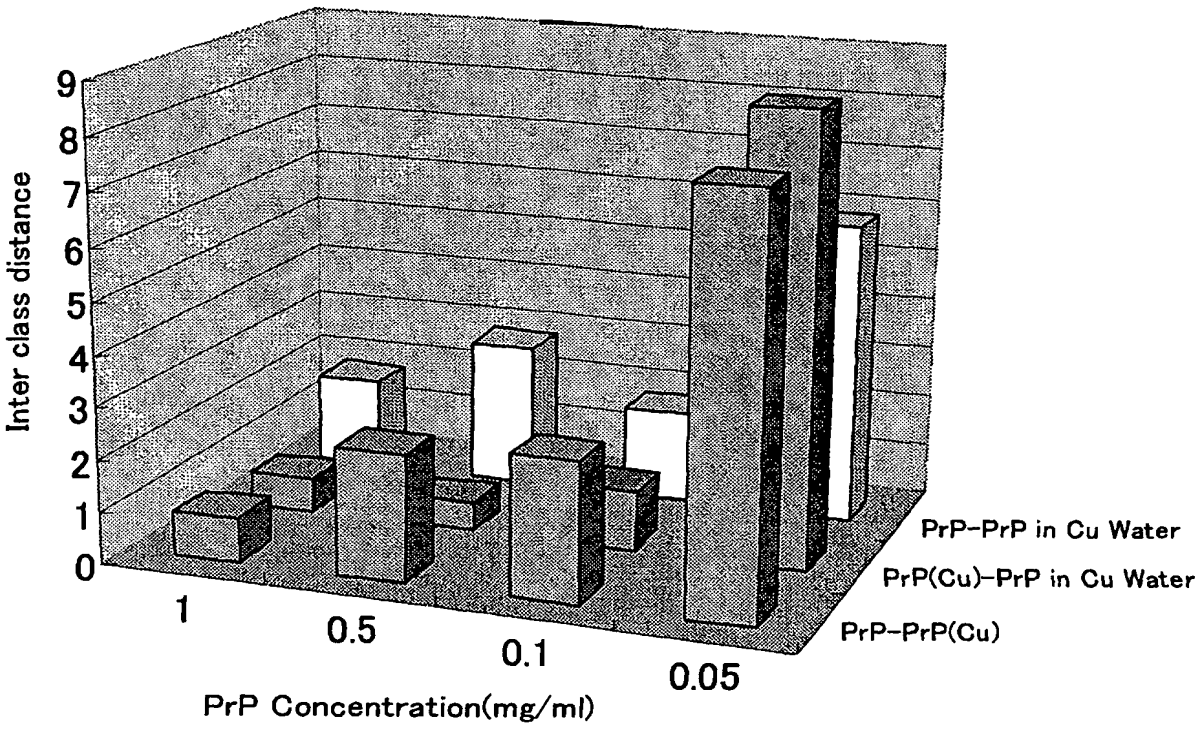
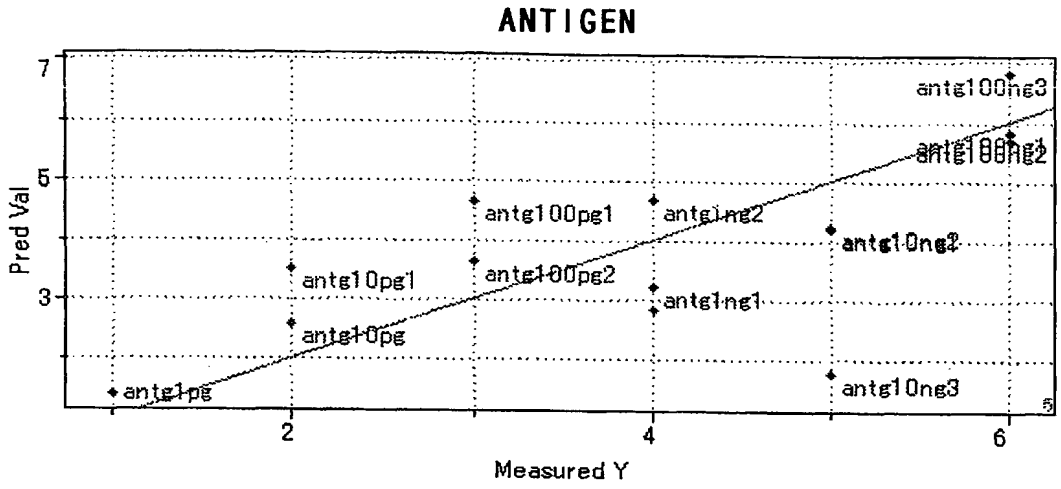


Fig. 22

(a)



(b)

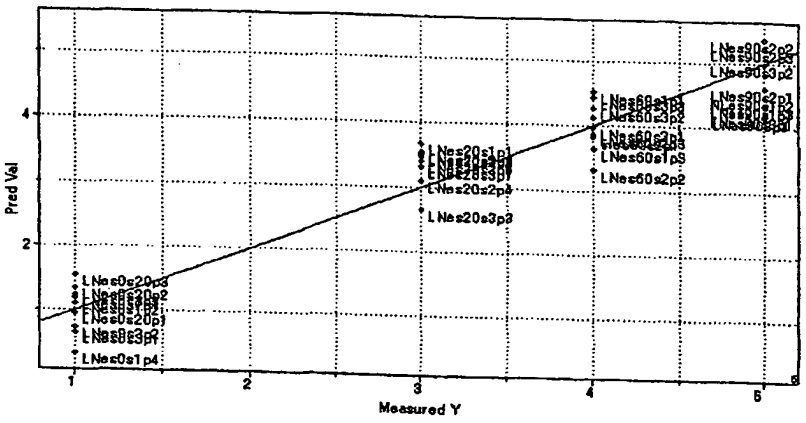
Factor9 (3回)	Percent	cumulative	SEV	Press Val	r Val	SEC	Press Cal	r Cal
	0.009203	99.94567	1.008785	14.24707	0.866991	0.026814	0.002876	0.999969
Factor5 (1回)	Percent	cumulative	SEV	Press Val	r Val	SEC	Press Cal	r Cal
	1.745422	99.94188	3.558607	88.64576	0.85991	0.41932	0.17583	0.99679

(c)

InterClassDistance (SIMCA, raw spectra, mean-center, smoothing 25nm)		PCA Factors
1	8.65	4
1&2	9.79	4
1&2&3	10.11	4

Fig. 23

(a)



(b)

Factor6 (3回)	Percent 0.116864	cumulative 99.8904	SEV 0.466675	Press Val 8.058082	r Val 0.951239	SEC 0.379212	Press Cal 4.314054	r Cal 0.973881
Factor5 (1回)	Percent 6.582126	cumulative 98.31849	SEV 0.937039	Press Val 3.512166	r Val 0.893979	SEC 0.357026	Press Cal 0.127468	r Cal 0.992689

Fig. 24

(a)

SIMCA DISTANCE of Granul/Powder Coffee serially diluted with water

CONCENTRATION AFTER DILUTION	SIMCA DISTANCE
1%	15.96
2%	5.98
3%	7.16
4%	6.77

(b)

SIMCA DISTANCE of Granul/Powder Sugar serially diluted with water

CONCENTRATION AFTER DILUTION	SIMCA DISTANCE
0.50%	5.15
1%	4.51
2%	7.6
4%	1.59

(c)

SUGAR Concentartion measurement,PLS regression (0.5,1,2,4%)

	Rv (Serial Dilution)	SEV (Serial Dilution)
Granul	0.995	0.0438
Powder	0.9998	0.0258

Fig. 25

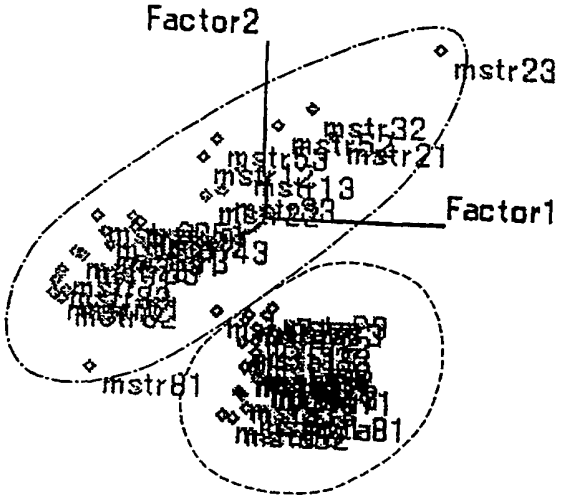


Fig. 26

Blood Plasma Spectra – Milk Component Estimation

Table 3-1. Relationship between first 10 principal components of blood plasma spectra and milk components

(a)

Parameter	min	max	average	The best way of data transf.	R
Fat, %	2.00	5.47	3.41	Log(1/T)	0.698
Crude Protein, %	2.88	4.05	3.32	D1	0.685
Casein, %	2.18	2.87	2.62	D1	0.728*
True protein, %	2.74	3.87	3.17	D1	0.683
MUN, %	1.40	3.10	2.00	Log(1/T)	0.546
Lactose, %	4.12	4.93	4.54	Log(1/T)	0.534

Statistically significant at: * P<0.05

Table 3-2. NIRS calibration and validation results for estimation of milk composition from the spectra of blood plasma by PLS regression

(b)

Parameter	The best way of data transf.	PLS factors	SEC	R	SECV
Fat, %	Log(1/T)	2	0.612	0.575	0.692
Crude protein, %	D1	4	0.208	0.829***	0.377
Casein, %	D1	6	0.108	0.938***	0.273
True protein, %	D1	4	0.133	0.863***	0.281
MUN, %	Log(1/T)	5	0.248	0.938***	0.584
Lactose, %	D1	3	0.177	0.596	0.239

Statistically significant at: *** P<0.001

Milk Spectra – Blood Plasma Component Estimation

Table 3-3. Relationship between first 10 principal components of milk spectra and some components of blood plasma

(c)

Parameter	min	max	average	The best way of Data transf.	R
Albumin, %	2.87	3.58	3.25	Log(1/T)	0.624
Glucose, mg/dl	45.9	72.7	61.6	Log(1/T)	0.361
BUN, %	11.3	21.2	15.9	Log(1/T)	0.618

Table 3-4. NIRS calibration and validation results for estimation of blood plasma composition from the spectra of milk by PLS regression

(d)

Parameter	The best way of data transf.	PLS factors	SEC	R	SECV
Albumin, %	Log(1/T)	7	0.174	0.718**	0.202
Glucose, mg/dl	Log(1/T)	4	4.588	0.322	4.691
BUN, %	D1	8	1.771	0.682*	1.969

Statistically significant at: * P<0.05 ** P<0.01

Fig. 27

Rumen Juice Spectra – Milk Component Estimation

Table 4-1. Relationship between first 10 principal components of rumen juice spectra and milk components

(a)

Parameter	min	max	average	The best way of Data transf.	R
Fat, %	2.00	5.47	3.41	D1	0.750*
Crude Protein, %	2.88	4.05	3.32	D2	0.703
Casein, %	2.18	2.87	2.62	D2	0.826**
True protein, %	2.74	3.87	3.17	D2	0.698
MUN, %	1.40	3.10	2.00	Log(1/T)	0.665
Lactose, %	4.12	4.93	4.54	D1	0.593

Statistically significant at: * P<0.05 ** P<0.01

Table 4-2. NIRS calibration and validation results for estimation of milk composition from the spectra of rumen juice by PLS regression

(b)

Parameter	The best way of data transf.	PLS factors	SEC	R	SECV
Fat, %	Log(1/T)	5	0.455	0.766***	0.583
Crude protein, %	D2	4	0.138	0.890***	0.231
Casein, %	D2	5	0.091	0.902***	0.191
True protein, %	D2	4	0.139	0.826***	0.241
MUN, %	Log(1/T)	7	0.161	0.942***	0.393
Lactose, %	Log(1/T)	3	0.204	0.283	0.232

Statistically significant at: *** P<0.001

Milk Spectra – Rumen Juice Component Estimation

Table 4-3. Relationship between first 10 principal components of milk spectra and some components of rumen juice

(c)

Parameter	min	max	average	The best way of Data transf.	R
PH	5.4	6.5	6.27	Log(1/T)	0.515
NH_3-N	2.2	18.8	8.42	Log(1/T)	0.516
C_2	50.4	64.6	58.6	Log(1/T)	0.555
C_3	16.9	36.1	23.1	Log(1/T)	0.532
C_4	11.1	19.0	14.7	Log(1/T)	0.457

Table 4-4. NIRS calibration and validation results for estimation of rumen juice composition from the spectra of milk by PLS regression

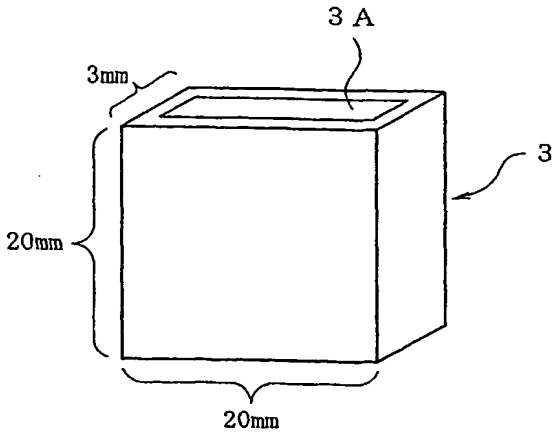
(d)

Parameter	The best way of data transf.	PLS factors	SEC	R	SECV
PH	Log(1/T)	4	0.26	0.471	0.27
NH_3-N	Log(1/T)	7	3.70	0.649*	4.22
C_2	Log(1/T)	7	3.02	0.692**	3.56
C_3	Log(1/D)	7	3.48	0.686*	4.06
C_4	Log(1/T)	6	1.71	0.569	1.89

Statistically significant at: * P<0.05 ** P<0.01

Fig. 28

(a)



(b)

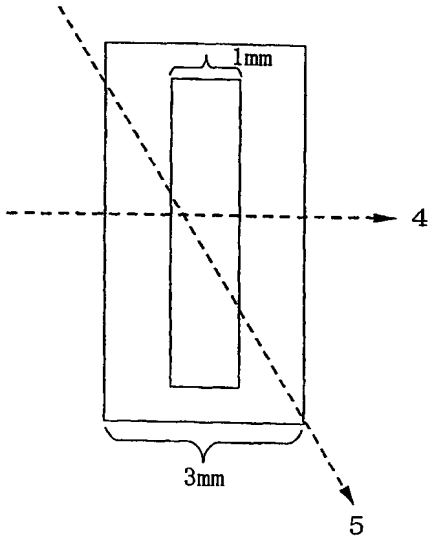
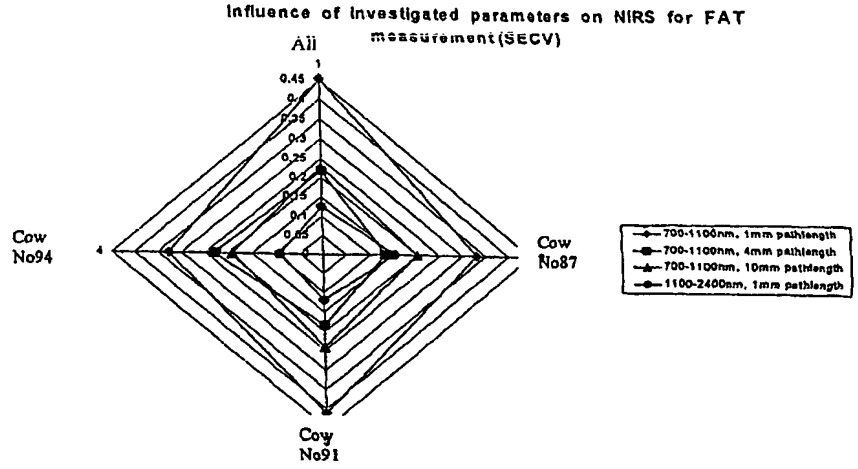
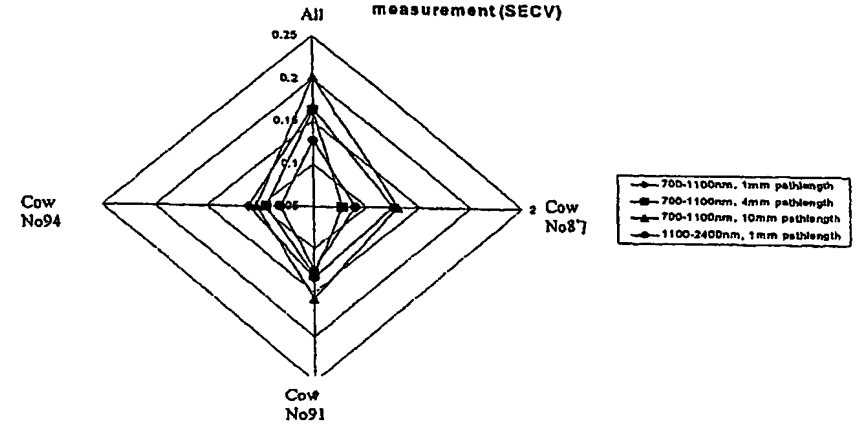


Fig. 29

(a)


Influence of investigated parameters on NIRS for FAT measurement (SECV)
All
Cow No94
Cow No87
Cow No91
700-1100nm, 1mm pathlength
700-1100nm, 4mm pathlength
700-1100nm, 10mm pathlength
1100-2400nm, 1mm pathlength

(b)


Influence of investigated parameters on NIRS for PROTEIN measurement (SECV)
All
Cow No94
Cow No87
Cow No91
700-1100nm, 1mm pathlength
700-1100nm, 4mm pathlength
700-1100nm, 10mm pathlength
1100-2400nm, 1mm pathlength

(c)

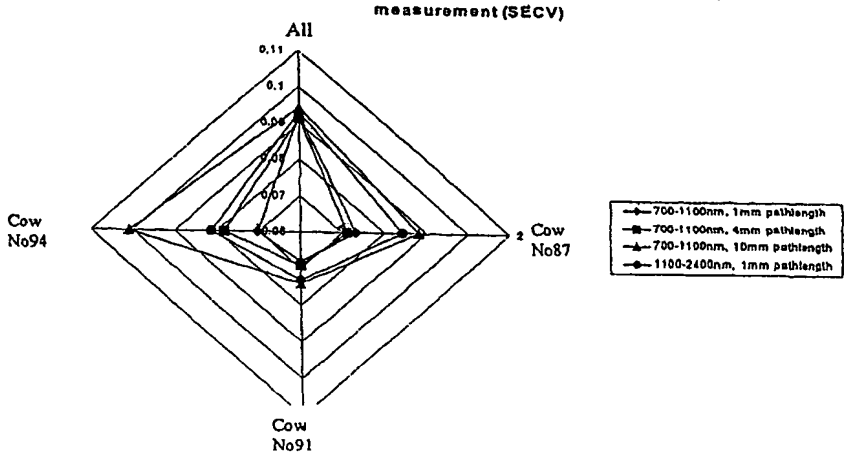
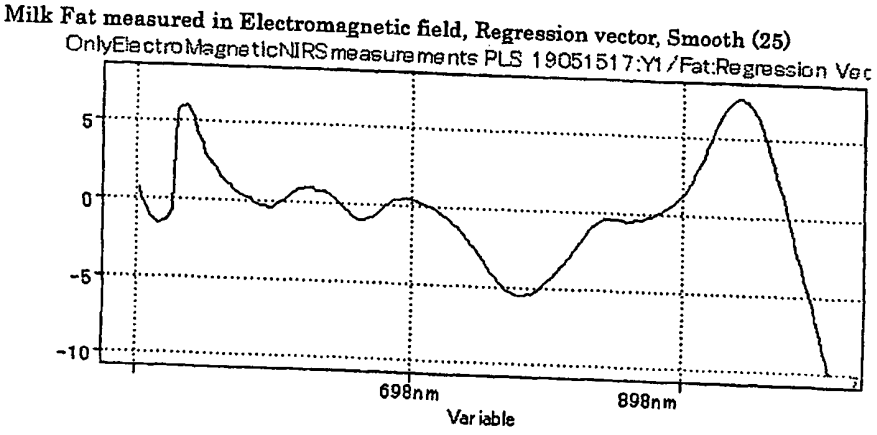

Influence of investigated parameters on NIRS for LACTOSE measurement (SECV)
All
Cow No94
Cow No87
Cow No91
700-1100nm, 1mm pathlength
700-1100nm, 4mm pathlength
700-1100nm, 10mm pathlength
1100-2400nm, 1mm pathlength

Fig. 30

(a)

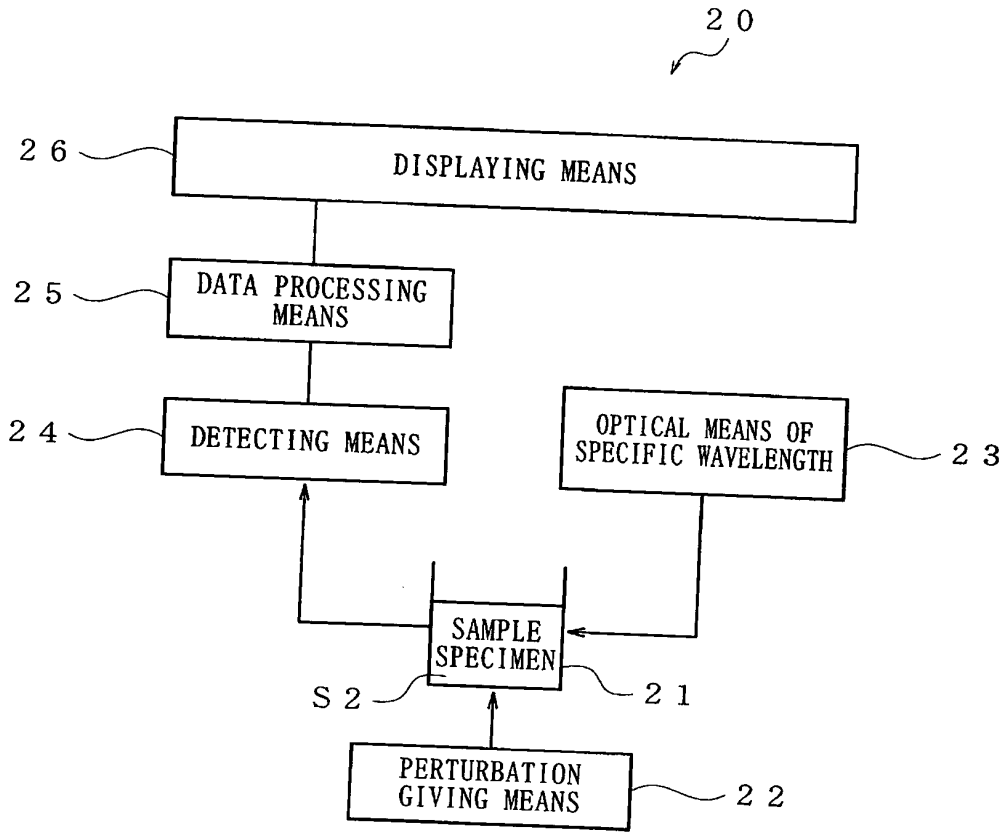


Important Wavelengths: 534nm, 620nm、688nm、694nm、778nm、844nm、858nm、940nm

(b)

	Factors	SEV	r Val	SEC	r Cal
Without EMF	Factor10	0.204269	0.980037	0.136665	0.994630
After Applying EMF	Factor9	0.087212	0.996256	0.067217	0.998611
In the presence of EMF	Factor9	0.071528	0.997483	0.056339	0.999024

Fig. 31


20
26
DISPLAYING MEANS
25
DATA PROCESSING MEANS
24
DETECTING MEANS
OPTICAL MEANS OF SPECIFIC WAVELENGTH
23
SAMPLE SPECIMEN
S2
21
PERTURBATION GIVING MEANS
22